Uncertainty Quantification and Multiscale Materials Modeling

June 13 -15, 2011

Eldorado Hotel and Spa, Santa Fe, New Mexico

Monday, June 13th

Session 1: **Statistics in Complex Physics Models** [Chair: Frank Alexander]

8:00 AM: *Breakfast Speaker*: **Ed Kober** *(LANL),* "Workshop Introduction"

8:30 - 9:20 AM   **Allen Robinson** *(Sandia)* "Fundamental Issues in the Representation and Propagation of Uncertain Equation-Of-State Information in Shock Hydrodynamics"

9:20 – 10:10 AM   **Krishna Rajan** *(Iowa State University)* "Multiscale Materials Modeling with the Right Stuff Data Mining to Rank Information"

10:10 – 10:40 AM   **BREAK**

10:40 – 11:10 AM   **Hany Abdel-Khalik** *(NCSU)* "Hybrid Framework for Enabling Uncertainty Quantification in Multi-Scale Multi-Physics Model"

11:10 – 11:40 AM   **Marian Anghel** *(LANL)* "Hierarchical, Multiscale, Spatio-Temporal Models for Material Structures and their Dynamic Interactions"

11:40 – 12:10 PM   **Ulisses Braga-Neto** *(Texas A&M)* TBA

12:10 – 1:10 PM   **LUNCH --- Session summary discussion** [Lead: Frank Alexander]

Session 2: **UQ Issues for Polycrystalline Materials** [Chair: Curt Bronkhorst]

1:10 – 2:00 PM   **Nicholas Zabaras** *(Cornell)* "Uncertainty Quantification and Predictive Modeling in Heterogeneous Media and Polycrystalline Materials"

2:00 – 2:50 PM   **Somnath Ghosh** *(Johns Hopkins University)* "Multi-Time Scaling Image Based Crystal Plasticity FE Models Dwell Fatigue Initiation in Polycrystalline Ti Alloys"

2:50 – 3:20 PM   **BREAK**

3:20 – 3:50 PM	**Curt Bronkhorst** *(LANL)* "Models for the Large Plastic Deformation Response of Polycrystalline Metals"
3:50 – 4:15 PM	**Andrew Richards** *(Caltech)* "Interplay Between Slip and Transformation Induced Deformation in Polycrystalline Solids"
4:15 - 4:45 PM	**Jeff Simmons** *(AFRL)* "Some Considerations When Linking Experimental Data with Simulations"
4:45– 5:10 PM	**Stephen Niezgoda** *(LANL)* "Quantification of Microstructural Variance: A modeling and experimental approach"
5:10 – 5:30 PM	**Session summary discussion** [Lead: Curt Bronkhorst]

Tuesday, June 14th

Session 3: **Integrated UQ Methodologies** [Chair: Mike Rogers]

8:00 AM:	*Breakfast Speaker:* **Blas Uberuaga** *(LANL)* "An Overview of the Materials Performance Optimization Focus Area within the Consortium for Advanced Simulation of Light Water Reactors (CASL)"
8:30 - 9:20 AM	**James Holloway** *(University of Michigan)* "Uncertainty in Shock Location in a Radiation Hydrodynamics Simulation Calibration, Tuning and Discrepancy"
9:20 – 10:10 AM	**Jon Woodring** *(LANL)* "Visualizing and Analyzing Uncertainty of Large Data Set"
10:10 – 10:40 AM	**BREAK**
10:40 – 11:10 AM	**Jayathi Murthi** *(Purdue)* TBA
11:10 – 11:40 AM	**Timothy Wallstrom** *(LANL)* "Quantification of margins"
11:40 – 12:10 PM	**James Langenbrunner** *(LANL)* "Uncertainty Qualification Estimating Uncertainty Due to Inference"
12:10 – 1:10 PM	**LUNCH --- Session summary discussion** [Lead: Mike Rogers]

Session 4: **UQ Issues for Atomistic Modeling** [Chair: Neil Henson]

1:10 – 2:00 PM   **Alejandro Strachan** *(Purdue)* "Multiscale Materials Modeling Applied to MEMS Devices"

2:00 – 2:50 PM   **Scott Shell** *(UCSB)* "The Relative Entropy as a New Framework for Multiscale Modeling and Coarse Graining"

2:50 – 3:20 PM   **BREAK**

3:20 – 3:50 PM   **Habib Najm** *(Sandia)* "Uncertainty Quantification in Multiscale Atomistic-Continuum Models"

3:50 – 4:20 PM   **Peter Schultz** *(Sandia)* "Modeling Nuclear Waste form Performance in NEAMS Strategy for Upscaling from Atoms Into Continuum"

4:20 – 5:00 PM   **Edward Kober** *(LANL)* " Ideas on Quantifying MD simulations"

5:00 – 5:30 PM   **Session summary discussion (***Lead: Neil Henson***)**

7:00 PM   **DINNER --** *Dinner Speaker**: Cris Barnes** (LANL)* "The MaRIE Concept*"*

Wednesday, June 15th

Session 5: **Other Uncertainties** [Chair: Francois Hemez]

8:00 AM: *Breakfast Speaker**: Francois Hemez** (LANL)*

8:20 - 9:00 AM   **Clint Scovel** *(LANL)* "Optimal Uncertainty Quantification-I"

9:00 – 9:40 AM   **Houman Ohwadi** *(Caltech)* "Optimal Uncertainty Quantification-II"

9:40 – 10:30 AM   **Tim Wildey** *(Sandia)* "A Posteriori Error Analysis of Stochastic Differential Equations Using Polynomial Chaos Expansions"

10:10 – 10:40 AM   **BREAK**

10:40 – 12:00 PM   **Session and workshop summary discussion (***Lead: Francois Hemez***)**

12:00 PM   **LUNCH --- Summary discussion continued**

1:00 PM   **Workshop adjourns**